

Key attributes of a modern statistical computing tool

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Abstract

In the 1990s, statisticians began thinking in a principled way about how computation could support statistics and statistics education. Since then, the pace of software development has accelerated, advancements in computing and data science have moved the goalposts, and it is time to reassess. Software continues to be developed to help do and learn statistics, but there is little critical evaluation of the resulting tools, and no accepted framework with which to critique them. In this paper, we present a set of attributes necessary for a modern statistical computing tool. This framework is designed to be broadly applicable to both novice and expert users, but the particular focus is on making a more supportive statistical computing environment.

A modern statistical computing tool should be accessible, provide easy entry, privilege data as a first-order object, support exploratory and confirmatory analysis, allow for flexible plot creation, support randomization, be interactive, include inherent documentation, support narrative, publishing, and reproducibility, and be flexible to extensions. Ideally, all these attributes could be incorporated into one tool, supporting users at all levels, but a more reasonable goal is for tools designed for novices and professionals to ‘reach across the gap,’ taking inspiration from each others’ strengths.

Keywords: Software design, Software evaluation, Exploratory data analysis, Data visualization, Randomization, Bootstrap, Reproducibility

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INTRODUCTION

Tools shape the way we see the world, and statistical computing tools are no exception. The affordances systems provide for building graphics, representing data, and modifying analysis all impact how users conceive of their statistical products. Often, a distinction is made between professional and educational tools, and the users of those tools have different goals and needs. However, no matter a user’s level of expertise, they can benefit from more flexible, powerful, and intuitive tools. As our world becomes increasingly data-driven, it is important to critically examine the tools we are using and look toward the future of computational possibilities.

The use of the term ‘tool’ to mean computer software or a programming language harkens to a future where computers do more than just amplify human abilities: they also augment them (Pea, 1985). In the same way objects we traditionally think of as tools (e.g., hammers, levers, and sewing machines) allow us to do much more than we can do on our own, computers can allow humans to ‘see’ and ‘think with’ data in higher dimensions and with more clarity than they otherwise could.

Historically, statistical computing tools have been sharply delineated into tools for learning and tools for doing statistics (McNamara, 2015; Baglin, 2013). This paper does not focus specifically on existing tools, although it draws heavily on McNamara (2016), which describes the current landscape of statistical computing. When tools for learning statistics are mentioned in this paper, the most common examples will be TinkerPlots and Fathom, two interactive tools for statistics education (Konold and Miller, 2005; Finzer, 2002). Most references to professional tools will be to the programming language R (R Core Team, 2016).

Interestingly, while statisticians have thought and written about principles underlying the tools for learning statistics, almost no critical work has been done to evaluate professional tools for doing statistics. In the educational context, Rolf Biehler’s 1997 paper *Software for Learning and for Doing Statistics* outlined principles for a statistical computing tool that would support novices in learning statistics and data analysis (Biehler, 1997). It provided a framework for the assessment of statistical software and called for statisticians to develop software for use in statistics education. The problems and ideas from

Biehler (1997) were used to drive the development of TinkerPlots and Fathom. The motivation and criticism of professional tools is much less rich, and tends to focus on language properties (Ihaka and Gentleman, 1996; Morandat et al., 2012).

We aim to generate a list of attributes that captures the necessary features for tools for both novices and professionals. Hopefully, these attributes can be used to frame critical discussions of statistical computing tools of all types.

Although we are satisfied with some features of existing tools, most have been around for many years, during which the computational landscape has changed. So, in addition to broadening the critical narrative to include professional tools, we would also like to update the criteria for assessment. In the 20 years since Biehler (1997), the nature of data has changed, with more data generated from a huge variety of sources (smart TVs, road sensors, personal fitness devices, and many more), streaming on the web, and heavily linked and aggregated (Dumbill, 2012; Lazar, 2013). As computer capabilities have improved, bigger data has become available locally, and the connection to cloud-based big data services are more accessible (Kandel et al., 2011). This explosion of data has generated more problems: critical (boyd and Crawford, 2012), technical (Tufekci, 2014), and pedagogical (Gould, 2010). Science has begun to focus more on reproducibility, and many statisticians are at the forefront of the associated computational work (Gentleman and Temple Lang, 2007; Nolan and Temple Lang, 2007; Xie, 2014). While statisticians often feel ‘data science’ is really just a term for statistics, the changes in data and science associated with the rise of computers do seem to afford new consideration (Donoho, 2015).

These changes compel statisticians to think critically about the tools they use. This paper outlines a list of 10 key attributes for a modern statistical computing tool. The attributes aim to be as broad as possible, encompassing the needs of novices and professionals, but they are focused specifically on the development of more supportive environments.

Often, programming languages are designed around goals of speed, efficiency, and compactness. These goals can result in extremely terse code that is difficult or impossible for humans to read.

Statistical computing tools require different goals. Statistics is rooted in the context of data, so it is important the results of an analysis (including the code that generated it)

be human readable. As demand for and interest in data analysis grows, we are trying to broaden the number of people who can work with data. To facilitate this, tools must support novices by being accessible and offering easy entry. However, even for experts, having transparent algorithms and providing interactive environments will improve productivity. No matter the user, a statistical programming tool should aim to make it easier for them to do and understand statistics.

We want to think particularly of novices, because if a tool is usable by novices it should be useable for everyone. The issues that face novices are similar whether the novice is in high school, college, graduate school, or a working professional picking up additional skills.

Although we are considering a broad range of users, it is useful to focus our discussion on “a user” rather than “the user” (Agre, 1995). For purposes of discussion, we will consider our target user to be a journalist looking to bring more computation into their work. Journalism has long embraced social science methods, with the first computer-assisted reporting institute launched in 1989 (Berret and Phillips, 2016). The changing nature of computers and the web has accelerated the field, however journalism schools have been slow to adapt to the ideas of data-driven journalism (Berret and Phillips, 2016). As a result, many journalists have limited experience with programming and statistics, but want to tell data-driven stories. They need to move from novices to producers very quickly. Journalists have a responsibility to expose others to the information they have discovered, so communication is one of their key goals. Since news publications have embraced the interactive web, journalists are at on the forefront of publishing modern, data-rich reports. Considering a data journalist as our target user means prioritizing tools that are easy to learn but also powerful and flexible.

Many of the ideas presented here are not new. In particular, these attributes attempt to distill principles and characteristics proposed by Rolf Bieher, Alexander Repenning, and John Tukey (Biehler, 1997; Repenning et al., 2010; Tukey, 1965), while also considering the recent developments in data and computing. John Tukey was considering the “technical tools of statistics” in 1965, and describing a vision for the future of statistical programming tools (Tukey, 1965). He argued statisticians should be looking for “More of the essential erector-set character of data-analysis techniques, in which a kit of pieces are available for

assembly into any of a multitude of analytical schemes,” more graphical and informal inference, “steadily increasing emphasis on flexibility and on fluidity,” and “greater emphasis on parsimony of representation and inquiry” (Tukey, 1965). Thirty years later, Rolf Biehler was thinking even more specifically about tools for novices. He defined three primary problems, the “complexity of tool problem” (existing tools were too hard to for novices to learn), the “closed microworld problem” (learning tools were designed for one particular type of problem or data set and couldn’t be extended) and the “variety problem” (because of the closed microworld problem, it was necessary to use many tools to do everything an instructor wanted to cover) (Biehler, 1997). Most recently, Alexander Repenning, David Webb, and Andri Ioannidou outlined the six requirements for a “computational thinking tool,” including having a low threshold, a high ceiling, and being equitable (Repenning et al., 2010).

A survey of statistical computing tools (McNamara, 2016) helps ground these ideas in the existing computational landscape. Considering the various positive qualities of current tools for doing and teaching statistics alongside Biehler’s goals (Biehler, 1997) and combining them with ideas from Repenning et al. (2010) and Tukey (1965), we developed a list of 10 attributes for a modern statistical computing tool. These are summarized in Table 1.

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| <ol style="list-style-type: none"> 1. Accessibility 2. Easy entry for novice users 3. Data as a first-order persistent object 4. Support for a cycle of exploratory and confirmatory analysis 5. Flexible plot creation 6. Support for randomization throughout 7. Interactivity at every level 8. Inherent documentation 9. Simple support for narrative, publishing, and reproducibility 10. Flexibility to build extensions |
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Table 1: Summary of attributes

Each requirement will be discussed in more detail in its respective section.

1 Accessibility

Tools should always be accessible, particularly to learners. As a baseline requirement, the software must be affordable (or free) and work with a variety of operating systems (Dunham and Henessy, 2008; Reppenning et al., 2010). In this context, most tools for teaching are accessible, because they are designed to work across platforms and are priced inexpensively. However, professional tools tend to be incredibly expensive and inaccessible for non-professional or occasional users. They are not accessible for small newspapers, nonprofits, individuals, or K-12 school systems.

Users in these contexts must consider if they have the funding for a tool, if it will work on the computers they have access to, and if they have the user privileges to install software. System administrators can be few and far between in newsrooms and underfunded school systems, so often the easiest way to ensure accessibility is to create a web-based tool. Cloud services allow users to access software from any machine with internet access, almost without regard for the operating system or version.

Beyond the accessibility of a tool to the masses, it is also important to consider the needs of people with disabilities. For a tool to be required in public schools, it must be compatible with accessibility features on modern computers (Office of the Chief Information Officer, 2001). Some progress has been made on programming languages accessible for blind users (Stefik et al., 2011; Godfrey, 2013), but given that many educational tools are visual, it is not clear if any of them are accessible to blind users. Of course, there are other disabilities that can impact a person’s ability to use a tool. Considering “universal design” (Connell et al., 1997) should be a component to any new statistical computing tool.

2 Easy Entry For Novice Users

Tools to be used by novices — and really, all tools — should make it easy to get started. This attribute comes directly from Reppenning et al.’s work on tools for computational thinking (Reppenning et al., 2010). It should be clear what the tool does, how to use it, and what the most salient components are. The tool should provide immediate gratification, rather than a period of frustration eventually leading to success.

Easy entry means users should be able to jump directly into ‘doing’ data analysis without having to think about the minutiae of the way data is structured in the system or the name of a plot type. We want novices to be able to begin exploratory data analysis within the first 10-15 minutes of using a tool.

Biehler argued, “In secondary education, but also in introductory statistics in higher education, using a command language system is problematical. We are convinced that a host system with a graphical user interface offers a more adequate basis” (Biehler, 1997). By Biehler’s estimation, a system providing easy entry for novices will likely have a visual component, either initially or throughout.

Indeed, visual tools like TinkerPlots and Fathom allow novices to create linked plots and multivariate data visualizations within the first minute of beginning the software. However, curriculum development using the programming language R has begun to put first emphasis on exploratory data analysis, rather than data structures (Pruim et al., 2014), so these goals can also be achieved in a scripting context. Given the success of the blocks-based language Scratch in computer science education (Resnick et al., 2009), it seems possible that a graphical system abstracting away syntax issues would be better for novices. However, there are many other ways easy entry can be achieved.

3 Data as a First-Order Persistent Object

A data analysis tool must necessarily deal with data. A tool cannot be considered to be designed for statistical computing if it does not make data one of its primary objects of interest. The way data are formatted and represented within the system is also of crucial importance. In this context, formatting and representation refer specifically to how the data appear to the user, not how they are stored within the computer’s memory system.

Modern data analysis tools should make it easy to access common data types (flat files, hierarchical data formats, APIs, etc.) and ‘see’ the full data (whether in a format allowing for value-reading or a higher-level view). Data should be a persistent object, with a reproducible workflow of wrangling to take raw data to clean.

3.1 Rectangular versus hierarchical data

Analysts are typically accustomed to thinking of data in a tidy rectangular format, composed of rows and columns or observations and variables. Rectangular data can be considered ‘tidy’ if every row represents one case (e.g., a person, gene expression, or experiment), and every column represents a variable (i.e., something measured or recorded about the case) (Wickham, 2014a). Tidy data are often visualized as a spreadsheet, and spreadsheets are the most common way people around the world interact with data (Bryan, 2016).

Interestingly, novices who have not encountered data before often do not use rectangular formats to represent their data, but rather default to a list-based or hierarchical format (Lehrer and Schauble, 2007; Finzer, 2013, 2014). So, although rectangular data has become prevalent, it may not be the most natural format. There are many hierarchical and list-based formats like JSON and XML which are used commonly on the web. These types of data are important for data science (Nolan and Temple Lang, 2014). However, they may require the development of new visual metaphors because the tidy rectangle will no longer suffice.

3.2 Viewing data

Many tools (including spreadsheets) make a view of the data the primary focus. In conversations with data journalists, they often mention scrolling through a spreadsheet, ‘reading’ the data values as their first line of inquiry. In contrast, programming languages like R and Python have traditionally not shown data to users when it is read in, instead requiring the use of function calls to view the first few rows of the data. This can be a sticking point for users transitioning from spreadsheet programs, so Integrated Development Environments providing a data preview have become popular (RStudio Team, 2014).

Whether provided by default or requested by the user, most current tools provide data to users in such a way that they can immediately read each individual value. However, there are other ways to ‘see’ an entire data set. For example, Victor Powell’s CSV Fingerprint project creates a colored image as a high-level overview of the data (Powell, 2014). Colors indicate data types (to see whether it is mostly numeric, categorical, integer, etc) and missing data (Powell, 2014). Again, more thought should be given to the visual metaphors

used to represent raw data in a system.

3.3 Sanctity of data

Another important consideration is how easy it is to modify the original data file. Raw data files should be kept in their original form to support reproducibility (Ball and Medeiros, 2012; Wilson et al., 2016). R uses data as its primary object and makes it difficult to modify the original data file. The affordances of R promote working with a copy of the data and creating a reproducible workflow of data cleaning. This paradigm implicitly values original data. In contrast, Excel does not privilege data as a complete object. Once a user has a spreadsheet of data open, modification is just a click or errant keystroke away, and the original value is lost forever. Because Excel does not keep a history of actions taken, there is no way to document changes.

3.4 Results as data

A system privileging initial data should also have a commitment to providing data as the result of all actions. In systems like SPSS, results are often text outputs that cannot be saved or incorporated into additional stages of the analysis. In SAS software and R, almost every result is itself data that can be used again. This was a design decision on the part of the language architects, and could be implemented in other systems. Tools of the future should follow suit, making all results re-useable data.

4 Support for a Cycle of Exploratory and Confirmatory Analysis

Statistical thinking tools should promote exploratory analysis, and its twin, confirmatory analysis. The complementary exploratory and confirmatory cycles were suggested by John Tukey in his 1977 book, and have been re-emphasized by current educators (Tukey, 1977; Biehler et al., 2013). The use of the term ‘cycle’ indicates how cyclical the data analysis process is. Each step can lead back to prior steps. The cycle can include generating statistical

questions, collecting data, analyzing data, and interpreting results (Carver et al., 2016). Hadley Wickham lists `import`, `tidy`, `transform`, `visualize`, `model`, `commutate` (Wickham, 2014b). In a pedagogical setting, educators often talk about the PPDAC cycle: Problem, Plan, Data, Analysis, Conclusions, typically attributed to Wild and Pfannkuch (1999).

Analysis cycles can be exploratory or confirmatory, and the two complement each other. If users find something interesting in a cycle of exploratory analysis, they need to follow with confirmatory analysis. The idea of EDA is to explore data deeply by computing simple descriptive statistics and making many simple graphs — of one variable or several — to look for trends. Although EDA can appear subjective, it sometimes comprises the best and richest method for analysis, particularly for finding patterns in the data and performing informal inference (Makar and Rubin, 2014; Rubin et al., 2006). Exploratory data analysis can also be used in the context of statistical modeling (Gelman, 2004).

The difference between exploratory and confirmatory analysis (or informal and formal inference) is like the difference between sketching or taking notes and the act of creating the final painting or writing an essay. One is more creative and expansive, and the other tries to pin down the particular information to be highlighted in the final product. A system supporting exploration and confirmation should provide a workflow connecting these two types of activities. Users need ‘scratch paper’— a place to play without the results being set in stone. While data analysis needs to leave a clear trail of what was done so someone else can reproduce it, a scratch paper environment might allow a user to perform actions not ‘allowed’ in the final product, like moving data points. Biehler called this capability ‘draft results’ (Biehler, 1997).

The ability to make many explorations in the data is akin to the charrette process in art. Charettes allow artists to provide provocations instead of prototypes (Bardzell et al., 2012). Provocations drive thinking forward, while prototypes tend to lock in a particular direction. In the context of data analysis, a system that could save many analyses in parallel ‘worlds’ to allow the user to look through the collection might provide provocations to the cycle of analysis.

For inspiration about how to link exploratory and confirmatory analysis, the book “Infographic Designers’ Sketchbooks” provides a glimpse into how designers of infographics

and data visualizations work (Heller and Landers, 2014). Designers of infographics typically start with pen-and-paper sketches, and use digital tools as digital paint. In contrast, designers of visualizations grounded in data (e.g., Mike Bostock, Tony Chu, Cooper Smith, Moritz Stefaer) begin by ‘sketching’ using code. They use a variety of computer tools to do this (e.g., Bostock’s sketches look to be done in R, Smith sketches in **Processing**), but they do not explicitly map color to paper the way the infographic designers do (Heller and Landers, 2014).

Many current systems for teaching statistics provide rapid exploration and prototyping (allowing users to manipulate data or play with graphic representations), but typically do not support the more formal final analysis. In contrast, professional tools tend to make it difficult to play with data (in R, creating multiple graphs takes effort, as does modifying parameter values), and they may not support cyclical exploration or rapid plot generation. Again, this is limiting, as a sense of play and discovery is important to data analysis. Data scientists repeatedly cycle back through questioning, exploration, and confirmation or inference, so analysis is never a linear process from beginning to end. A statistical computation tools should support this cyclical process.

5 Flexible Plot Creation

To fully support data analysis (both exploratory and confirmatory), a tool needs to emphasize plotting. When Tukey wrote *Exploratory Data Analysis*, computers were not in everyday use, so his text suggests using pencil and paper to produce descriptive statistics and simple plots (Tukey, 1977). Today, the tasks listed in the book are even easier because of the many computer tools facilitating them, and the results are analogous to those made by hand. Indeed, some plot types popularized by Tukey (such as the boxplot) were designed to be easy for humans to draw, but computers now allow us to explore the same data in richer ways (like overlaid density plots). Simply being able to implement plots Tukey drew by hand in the 1970s is not enough; computers should be enabling even more powerful types of exploration.

Computational tools make it possible to visually explore large datasets in ways that would be difficult or impossible using just pencil and paper. For example, Jacques Bertin

developed a method for reordering matrices of unordered data in the 1960s. Bertin’s method involved cutting up paper representations of matrices or creating custom physical representations, then reordering the rows and columns by hand (Bertin, 1983). At the time, this method was laborious, but now (like the plots John Tukey developed by hand in the ‘60s) Bertin’s methods are easily implemented on the computer.

While having easy access to static plots is useful, a statistical computing tool should give humans capabilities they would not have otherwise. An exemplary method is the Grand Tour, which takes high-dimensional data and produces projections into a variety of 2- and 3-D spaces, walking a user through many views of their data to expose clusters and trends (Buja and Asimov, 1986). A simpler example that can also provide insight is the generalized pairs plot, which displays all 2-variable relationships in the data (Emerson et al., 2013). These plots allow humans to look for patterns in higher dimensions than they could ordinarily visualize.

Providing easy plotting functionality of many variables should be a goal of every tool, whether for learning or for doing statistics. Tools, particularly those for novices, must choose whether to provide a few simple plotting functions or the ability to fully customize graphics. While it can seem simpler to provide a small set of standard data visualizations, creating visualizations from primitives both provides more flexibility for the user and reinforces the mapping between data and aesthetics. Ideally, a statistical programming tool would make it simple to begin plotting (to facilitate EDA) and to produce standard graphics, while also allowing users to create novel plot types.

6 Support for Randomization Throughout

Computers have made it possible to use randomization and bootstrap methods where approximating formulas would once have been the only recourse. These methods are not only more flexible than traditional statistical tests, but can also be more intuitive for novices to understand (Pfannkuch et al., 2014; Tintle et al., 2012). Randomization and simulation can help make inference from data, even if those data are from small sample sizes or non-random collection methods (Efron and Tibshirani, 1986; Lunneborg, 1999; Ernst, 2004).

These methods have been gaining popularity in statistics research and trickling down to

the educational context as well. Several popular introductory statistics textbooks focus on randomization and simulation methods (Diez et al., 2014; Tintle et al., 2014; Lock et al., 2012), and other resources help get instructors up to speed (Hesterberg, 2015). These materials avoid the issue that many introductory statistics courses fall into, where the course can begin to feel like an infinite grab-bag of methods. Instead, they show randomization as a unifying method to answer many statistical questions using one framework.

The application of randomization and the bootstrap is a place where tools for teaching statistics shine. Popular applet collections provide simple randomization and bootstrap functionality (Chance and Rossman, 2006; Morgan et al., 2014). TinkerPlots and Fathom also provide intuitive visual interfaces for this (Finzer, 2002; Konold and Miller, 2005). However, professional tools have lagged behind. R provides the most complete functionality, but it is not always simple to use.

Randomization and the bootstrap can also be leveraged through the use of visual inference. Statisticians have been working on methods to use randomized or null data to provide graphical inference protocols (Wickham et al., 2010; Majumder et al., 2013; Buja et al., 2009). Humans are adept at finding visual patterns, whether the patterns are real or artifacts. Indeed, humans looking at graphs are often better than computers at identifying trends in data (Kandel et al., 2011).

Graphical inference helps people train their eyes to more accurately judge whether a pattern is real or not, and has been extended for use in validating models (Majumder et al., 2013; Buja et al., 2009; Gelman, 2004). Similar work has been done to use bootstrapped visualizations to provide a visual representation of uncertainty in a plot (Hullman et al., 2015), which can help highlight the potential for fallibility due to bias or sampling variation.

Because of their intuitive nature and generalizability, randomization and bootstrap methods can be helpful for novices and experts alike. They can be used in a variety of contexts, including graphical inference methods bridging the gap between exploratory and confirmatory analysis.

7 Interactivity at Every Level

To be interactive, a system must allow users to interact with it. The more direct the manipulation, the better. This means valuing pinch-zoom over a dropdown menu with an option for zoom, click-and-drag selection over a form allowing the user to enter filtering values, and linked plots and analysis over a set of disconnected products.

Interactivity is becoming standard on the web. Users of Google maps know they can pan and zoom a map, and Apple has strong opinions on which direction is more ‘natural’ to scroll. On smartphones we swipe left to reject a date, launch angry birds, drop pins on our location, and dismiss notifications with the flick of a finger.

To be relevant, data analysis platforms need to follow suit. For novices, we want to “Teach about, and with, interactive graphics” (Ridgeway, 2015) so they become adept at seeing data in this way. As Biehler suggests, we want to encourage direct manipulation rather than modifying a script (Biehler, 1997). Today, educational tools provide this type of direct manipulation, but professional programming tools do not. However, even textual programs can shorten the time between making a change in the code and seeing the results. Computer futurist Bret Victor has made shortening this loop one of his driving design principles, to provide users with the ability to see the direct results of their actions without waiting for something to compile (Victor, 2012).

In the context of statistical programming, Deborah Nolan and Duncan Temple Lang make the distinction between dynamic documents (those that are compiled and then automatically include the results of embedded code), and interactive documents (those that let a reader interact with components like graphics) (Nolan and Temple Lang, 2007). Given the goals of interactivity at every level, and the importance of publishing, the a modern statistical programming tool should provide ‘dynamic-interactive’ graphics. Users could interact with any component of the document and have the results update in realtime.

7.1 Levels of interactivity

Interactivity can take place at three levels. The first is in the context of developing an analysis. Ideally, users should be able to build their analysis using visual steps, as in drag-and-drop plot creation. Menus and wizards are a type of ‘interaction,’ but are not direct

interaction and don't add any intuition about the process.

The second level is within the analysis session, where all results should themselves be interactive. The tool should support graphs as an interface to the data (Biehler, 1997). Behaviors like brushing and linking should do dynamic subsetting (Few, 2010). All graphs should be zoomable, it should be easy to change the data cleaning methods and see how that change is reflected in the analysis afterward, and parameters should be easily manipulable. As Biehler suggests, tools should provide functionality for formatting, interacting with, and enhancing graphics (Biehler, 1997). Such simple parameter manipulation helps support exploratory data analysis.

The system should also make it possible to see multiple coordinated views of everything in the user's environment. Rolf Biehler suggests a multiple window environment to facilitate easy comparisons (Biehler, 1997). The importance of a coordinated view is supported by researchers who suggest allowing for multiple views of the same data may help people gain a more intuitive understanding (Shah and Hoeffner, 2002; Bakker, 2002). In many systems, this is supported by brushing and linking (Wilkinson, 2005).

Finally, the finished data product from the tool should be interactive. This goal means that the audience of a piece of data analysis— even if they do not know much about statistics — could play with the parameters and convince themselves the data were not doctored.

As may be expected, standalone educational tools do a better job of providing interactivity than professional tools.

TinkerPlots and Fathom highly interactive, allowing users to drag-and-drop variables onto their plots and supporting brushing and linking between plots. Highlighting cases in the data table highlights them in every plot. They make it easy to interactively develop analysis and play with it, but do not support sharing interactive results with someone who does not have the software.

On the other hand, interaction has historically been more challenging in professional tools. The history of statistical computing traces back to the pre-graphics era of computers, so most systems rely on static code. This paradigm means users are not incentivized to return to the beginning of the analysis to see how a code modification would trickle down.

And, even if a programmer wants to manipulate a parameter value in their code, they must modify the code and re-run it, making the comparison between states in their head. Comparing two states in this way may be possible, but comparing more than two is difficult. This is a cognitive burden we no longer need to put on users (Victor, 2012). If results were immediately accessible, it would make it possible to make hundreds of comparisons in just a few seconds.

In recent years, some of these possibilities have begun to emerge. ‘Notebook’ functionality in several environments allows a user to execute code chunks directly within their source file (Perez and Granger, 2015; RStudio Team, 2016). For experienced programmers, the production of interactive documents that respond to user input is possible (Chang et al., 2015; Bostock, 2013; Satyanarayan et al., 2016). While these packages allow expert users to create dynamic graphics, they are too complicated for a beginner.

As a result, most current published work with interactive abilities is the result of a bespoke process. Because few tools exist to facilitate the development of fully interactive data products, people who want to generate such products must hard-code them for a particular application. Two exemplary pieces of journalism include a simulation-based look at hurricane impacts in Houston by ProPublica, which allows readers to manipulate parameters of the simulation (Satija et al., 2016), and the IEEE programming language ratings (Cass et al., 2014) which provides access to the weight parameters used for each data source in the rating algorithm.

The power and usefulness of a truly interactive data analysis platform is easy to imagine. If all parameters were manipulable, it would be easier to get an intuitive sense of the parameter space, and therefore the fragility of a particular piece of an analysis.

In the case of a histogram, the bin size and width could be dynamically updated, providing an affordance for the manipulation of these parameters. If a user had used a cut point to create a categorical variable from a continuous variable, and then fed that categorical variable into a regression model, the system would allow them to manipulate the cut point to see the effect on regression parameters and interaction effects. When using a loess smoother, the span could be manipulated to show the variety of functions that would be fit.

8 Inherent Documentation

Systems should provide inherent documentation. In the words of Danny Kaplan, we want computing tools to “highlight the logic of what is going on.” (Kaplan, 2007). Most programming language documentation is hard for novices to comprehend, so we first want help that is helpful. However, the idea of a inherent documentation goes one step further, to help that is integrated into the process of using the tool. Instead of having to go to a second place to learn what a feature is or what a function does, those objects should provide documentation as a unified part of themselves.

Ideally, every component of a system should visually show the user what it is going to do, versus just telling them. However, even in textual languages, inherent documentation can be achieved by bringing the syntax of the language more in line with human language. Function names that say what they do are more valuable than those that preserve keystrokes. Supportive features like tab completion can make documentation of parameters more inherent to the analysis process.

For example, if a tool is going to perform k-means clustering, the basic level of documentation should be the words “k-means.” Ideally, the user should see a visual representation of the algorithm, and as it is applied to the data interim steps should be visualized (Mühlbacher et al., 2014). Of course, using a computer is not the same as moving through the real world, so interface designers must think carefully about visual metaphors that make the most sense. Sometimes, this means mimicking the real world (as in the desktop metaphor, with folder icons and a trash can) and sometimes developing a new visual language (as may need to happen for visualization of models, database operations, and the like). Interactive controls of a system should give some idea of what they are going to do, either by their design or by the presentation of ‘scented widgets’, embedded visualizations providing hints to users about what elements are capable of (Pousman et al., 2007).

9 Simple support for narrative, publishing, and reproducibility

One important component of data science is the communication of results in such a way that the audience understands them. We have already considered the importance of flexible plot creation, which is a form of visual communication. In addition to plots, almost all data analytic products require some form of narrative to accompany the work and contextualize it for readers. The products of a statistical computing system should be as easy to understand as the process of creating them, and they should be simple to share with others. Integrated narrative and button-click publishing will provide affordances that support reproducibility. Reproducible, interactive workflows may help to build confidence in results because they can be easily verified even by non-experts.

9.1 Narrative

Historically, analysis workflows have tended toward a paradigm of doing analysis in one document and narrative in another. Programmers typically separate the documentation of their code from the code itself (code comments notwithstanding). Data analysts often create their data analysis code first, then go back to create a narrative surrounding the analysis. Data journalists refer to the process of performing analysis in Excel and writing about the results in Word as keeping a ‘data diary.’

In contrast, a good statistical programming tool should have affordances to encourage narrative alongside or mixed in with the code to facilitate the integration of storytelling and statistical products. Donald Knuth calls this ‘literate programming’ because it is easier for humans to read and understand (Knuth, 1984).

The tools that do the best job at this allow users to write formatted text and delimited code, then process the document to create a final product with text, code, and code output (Perez and Granger, 2015; Xie, 2014).

However, even the best current tools leave something to be desired. They feel constrained, and do not lend themselves to the type of expressive work that characterizes data science. Delimiting code chunks is a fairly lightweight process, but it does require some

additional syntax. And including incidental numbers into narrative sentences can be tricky. A better solution would allow for explicit linking between code chunks (or, automatic detection of reactive connections), and the ability to drop any piece of an analysis into the text.

9.2 Publishing

Ideally, data analysis results and related products could be published with ease. Journalists could create a data-driven website, citizen scientists could share insights in the data they helped create with their friends and family, and people working together across an organization (or across the globe) could stay up-to-date on their collaborators' contributions. In all these scenarios, the publishing format should allow for exploration (discussed in more depth in Section 7). In fact, the ideal case would be a finished product allowing for full access to all the computation in the analysis. In this way, users could continue to explore the data, modify the analysis, and see the effects of their changes on the analysis and visualizations.

As the expected user base for analysis publication is wide (encompassing both novices and experts) the language the analysis is written in should be the same as the language it is published in. Currently, it is often necessary to translate from one format to another to share analysis. For example, a data journalist using RMarkdown to document their analysis will need to format it after the fact using their newspaper's content management system. To achieve the goal of native publishing, it is likely new linkage pipelines will need to be developed in order to streamline these transitions.

In data journalism, simple publishing abilities for fully interactive results of a data analysis could empower journalists to produce richer articles. Such articles could be accompanied by the reproducible code that produced them, allowing readers to audit the story. Similarly, as reproducibility becomes more valued in the academic community, data products are more often accompanied with fully reproducible code. If the code were interactive, it would widen the potential audience of the academic work.

9.3 Reproducibility

Reproducibility supports the aims of science, and should therefore be integrated with the work of data science (Buckheit and Donoho, 1995; Sandve et al., 2013; Ince et al., 2012; De Leeuw, 2009). Teaching novices to use tools that support reproducibility can help ensure it becomes an integral part of their statistical and data workflow (Carver et al., 2016).

There are many definitions of reproducibility. Here, we take a somewhat narrow view. A reproducible analysis is one that can be re-run (potentially years later, or by a different person) with the same data to produce exactly the same result. A slight extension to this is an analysis that can be re-run with a modified version of the original data to get analogous results (Kandel et al., 2011; Sandve et al., 2013; Broman, 2015). For example, the initial analysis was done on 2016 data but needed to be run again on 2017 data, or the initial analysis used corrupted data that should be replaced by a corrected version.

It may sound simple to achieve this goal. However, in practice there are many factors that make it challenging. Software versions can change, package dependencies can get broken, and—most disruptive to the process—authors often do not manage to document their entire process. They may have done data cleaning outside the main software package (e.g., the bulk of the analysis was done in R but the author did data cleaning in Excel before the analysis), or run analysis steps without adding them to the code document. They may provide out-of-date code, or code with bugs that need to be addressed before it will run. These problems can be at least partially addressed with tooling.

Integrated narrative and simple publishing will necessarily encourage reproducibility. If analysis developers are writing narrative as they write code, the results will be easier to interpret and more likely to be housed in the same place. If it is easy to publish this type of document, readers will have access to a richer version of the analysis than is typically shared. Therefore, the products of statistical computing tools should continue to become more reproducible.

However, there is a lot of work to be done before any statistical computing tools can be said to fully support the entire spectrum of reproducibility.

A fundamental feature supporting reproducibility is the ability to save the data analysis

process. Some teaching tools (e.g., applets) do not allow state to be saved in any way. In other systems, like Fathom and Excel, analysis is not reproducible because it was produced interactively. Even in 1997, Rolf Biehler was aware of this drawback to interactive systems; “It may be considered a weakness of systems like Data Desk that the linkage structure is not explicitly documented as it is the case with explicit programming or if we had written the list of commands in an editor. An improvement would be if a list of commands or another representation of the linkage structure would be generated automatically” (Biehler, 1997). Most interactive tools do allow the user to save the environment that produced the product, but do not document the steps taken within the environment. An independent researcher could use the saved document to explore the analysis, but may not be able to discover the steps to produce the final product. These types of tools also make it impossible to re-run the analysis on slightly different data.

Again, professional tools allowing for the integration of narrative and code are beginning to support some of these goals. Users can now author entire analyses within a single document, fulfilling Broman’s ‘everything with a script’ and ‘turn scripts into reproducible reports’ (Broman, 2015; Xie, 2014). Some of these tools are simple enough to be integrated in introductory college statistics courses (Baumer et al., 2014). However, even experts trying to implement reproducible workflows have found it difficult to fully document their process (FitzJohn et al., 2014; Garijo et al., 2013). For novices, full reproducibility is even more challenging (Garijo et al., 2013).

Future systems should therefore be designed in order to support reproducibility more fully. This may entail saving a version of the computer’s state, tracking all ‘scratch work’ alongside code put into a ‘final draft,’ automatically recognizing dependencies on files, packages, and custom functions, and providing a visual representation of those dependencies to the user. This vision would move close to Nolan and Temple Lang’s vision of dynamic, interactive documents (Nolan and Temple Lang, 2007).

10 Flexibility To Build Extensions

The flexibility to build extensions is necessary in order to prevent a tool from becoming obsolete. Users must be able to create new components of the system as methods are

developed, computers improve, or scientific discoveries are made. To be a computational thinking tool, building extensions is a required feature such that the system has a “high ceiling,” preventing users from ‘aging out’ or ‘experiencing out’ of a system (Repenning et al., 2010). In a statistical computing tool, it should be possible to develop new visualization types and data processes from other modular pieces.

Professional tools can be looked to for inspiration, because they tend make it easier to create new components of the system using old ones. R even has a centralized repository where other users can easily find and import others’ work (R Core Team, 2015). Of course, professional tools are harder to get started using, but they can look to tools for novices for inspiration on easy entry. Currently, the tools easiest for novices to use fail to provide a high ceiling, although Biehler argued that “adaptability (including extensibility) is a central requirement for data analysis systems to cope with the variety of needs and users” (Biehler, 1997).

Any system hoping to stay the test of time must provide the flexibility to build extensions. In a statistical computing tool, these extensions may be visual or computational, and should be written in the same language they are executed in.

11 CONCLUSION

This list of 10 attributes aims to encompass the most important qualities for a modern statistical computing tool. We have focused on an idealized data journalist as our target user, but we hope that the attributes are relevant to novices at a variety of ages as well as to professionals. More than anything, these attributes are designed to start a critical conversation about the design of statistical computing tools.

Considering the existing tools for statistical computing, McNamara (2016) suggests that none of them fulfill all the attributes outlined above. Most tools can be described as either a tool for learning statistics or a tool for doing statistics. Those for learning statistics tend to be better at accessibility, easy entry, exploratory data analysis, flexible plot creation, randomization, and interactivity. For example, the learning tools TinkerPlots and Fathom are highly interactive and intuitive, but make it difficult to share results. Spreadsheets like Excel are highly accessible to a broad audience across the world, but obscure the

computational processes taking place. In contrast, professional tools privilege data as a first-order object, consider flexible plot creation from another angle, support reproducibility, and have the flexibility to build extensions. A summary table of many popular statistical computing tools and how they satisfy the requirements is shown in Appendix 2. For more details, see McNamara (2016).

There are no currently-existing tools satisfying all the attributes, which suggests the need for new tools. It would be ideal to conceive of a single tool that could support users at all levels. For example, a blocks programming language with streamlined domain-specific language could step novices into more complex analysis. However, there are few examples of similar tools in other domains so it seems unlikely such a system will emerge.

If we acknowledge that users will likely have to move from one type of tool to another, software developers should be looking for ways to ‘bridge the gap’ between the two types of tools (McNamara, 2015). In other words, in tools with traditionally difficult learning curves, designers should consider how to lower the barrier to entry, while in tools where users tend to ‘experience out’, designers should build (either technically or pedagogically) an onramp toward the next tool. R has historically been difficult to get started using, but curricula and packages have been developed to lower the barrier to entry (Baumer et al., 2014; Pruim et al., 2014). Researchers have also begun studying instruction methods that best support learning of both statistics and statistical computing (Baglin, 2013). These efforts have not solved the problem of easy entry, but are easing the transition. More work needs to be done, but other tools could take inspiration from these initial efforts.

As new tools are developed and existing ones are refined, statistical practitioners need to remain actively engaged in their development and critique to ensure they can support learning as well as doing statistics. Hopefully, this paper can act as a guide as we begin to engage more fully with this conversation.

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A How current tools stack up

Table 2 outlines how many current tools do (or do not) illustrate the attributes outlined in this paper.

	Accessibility	Easy entry	Data as first-order object	EDA/CDA	Flexible plotting	Randomization	Interactivity	Inherent documentation	Narrative, publishing, reproducibility	Flexibility for extensions
Graphing calculators	*	✓								
Excel	*	✓					✓			
applets	*	✓				✓	✓			
TinkerPlots	*	✓		✓	✓	✓	✓	✓		
Fathom	*	✓		✓	✓	✓	✓	✓		
R	✓		✓	✓	✓	*	*		✓	✓
Python	✓		✓		*	*	*		✓	✓
SAS software			✓	✓		*			*	✓
Stata software			✓	✓		*			*	✓

Table 2: A summary of many currently-available tools for learning and doing statistics, and how they satisfy the attributes outlined in this paper. Asterisks indicate partial satisfaction of the attribute. For example, most tools are not accessible, either because of prohibitive cost or because they do not support disabled users. R and Python are free and can be used with adaptive technology. R, Python, SAS software, and Stata software get an asterisk for randomization because it is possible within the system, but difficult for novices. Similarly, R and Python can be used to create interactive graphics, but it is difficult, and SAS software and Stata software can be used to create reproducible reports, although it is difficult.